UCRL-CONF-222914

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

An Arbitrary Lagrangian Eulerian Formulation with Adaptive Mesh Refinement for Hydrodynamics and Material Modeling

P. Wang

July 17, 2006

7th World congress on Computational Mechanics
Los Angeles, CA, United States
July 16, 2006 through July 22, 2006

Disclaimer

An Arbitrary Lagrangian Eulerian Formulation with Adaptive Mesh Refinement for Hydrodynamics and Material Modeling

Ping Wang
Lawrence Livermore National Laboratory

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Outline

- Research areas and objectives
- Background and applications
- Mathematical formulation
- Numerical algorithm
- Technical approach
- Results and discussion
- Conclusions
- Future work

Research areas and objectives

- Dynamic ALE-AMR for hydrodynamics and material modeling: a numerical method combining an ALE formulation with AMR both in space and time – AMR meshes are dynamically generated during the simulation.
- Why ? Efficiency, accuracy, and possibility to solve problems that can not be solved by a single static mesh because of limits of our current computing resources or current methods.

Mathematical formulation for hydrodynamics and material modeling

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{U} \tag{1}$$

$$\frac{D\vec{U}}{Dt} = \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma} \tag{2}$$

$$\frac{De}{Dt} = \frac{1}{\rho} V (s_{11}\dot{\epsilon}_{11} + s_{22}\dot{\epsilon}_{22} + s_{33}\dot{\epsilon}_{33} + 2s_{12}\dot{\epsilon}_{12} + 2s_{23}\dot{\epsilon}_{23} + 2s_{31}\dot{\epsilon}_{31}) - P\dot{V} \tag{3}$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + U \cdot \nabla \tag{4}$$

$$\dot{\epsilon}_{i,j} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \tag{5}$$

$$s_{ij} = \sigma_{ij} + P\delta_{ij} \tag{6}$$

$$P = K(\frac{\rho}{\rho_0} - 1) \tag{7}$$

$$\dot{s}_{ij} = 2\mu\dot{\epsilon}_{ij} \tag{8}$$

Mathematical formulation for elastic and plastic flow and material model

$$\sqrt{2J} - \sqrt{2/3}Y \leq 0 \qquad (9)$$

$$Y = a(b + \varepsilon^{p})^{c}$$

$$2J = [s_{xx}{}^{2} + s_{yy}{}^{2} + s_{zz}{}^{2} + 2(s_{xy}{}^{2} + s_{yz}{}^{2} + s_{zx}{}^{2})]$$

Johnson-Cook damage model

$$\varepsilon f = \left[D1 + D2\exp\left(D3\frac{p}{\overline{\sigma}}\right)\right]\left[1 + D4\ln\left(\frac{\dot{\varepsilon}}{\varepsilon_0}\right)\right]\left[1 + D5\frac{T - Tr}{Tm - Tr}\right] \qquad (10)$$

ALE-AMR: Numerical algorithm

ALE:

Finite volume method with a predictor-corrector scheme for staggered variables on moving mesh

- Lagrange motion (Wilkins, Tipton, et al)
- Mesh relaxation (Winslow, Crowley, Jun, et al)
- Solution Remap (Colella, Van Leer, et al)
- Material modeling (Becker)

AMR:

- Adaptive gridding methods
- Dynamically, locally refined Cartesian meshes (Berger, Oliger, Colella, et al)

ALE-AMR:

- AMR on moving meshes for gas dynamics (Anderson, Pember, et al)
- ***AMR on moving meshes for elastic-plastic flow and material modeling***

ALE-Lagrange

Overall algorithm of Lagrange step: get t=n+1 from t=n :

Predictor

1. Compute the acceleration by using the momentum equations : an=f(xn,pn,sn,qn,h)/m
2. Integrate the velocity : up=un+dt*an
3. Integrate the node positions: xp= xn+0.5*dt*(un+up)
4. Compute the strain rates : r=f(un,up,xn,xp)
5. Compute the volume and densities: dp=dnVn/Vp
6. Compute the energies: ep=f(pn,qn,sn,r,h,Vp,Vn)
7. Compute the stresses: sp=f(sn,Vn,Vp,r)
8. Compute the pressure: pp=f(dp,ep)

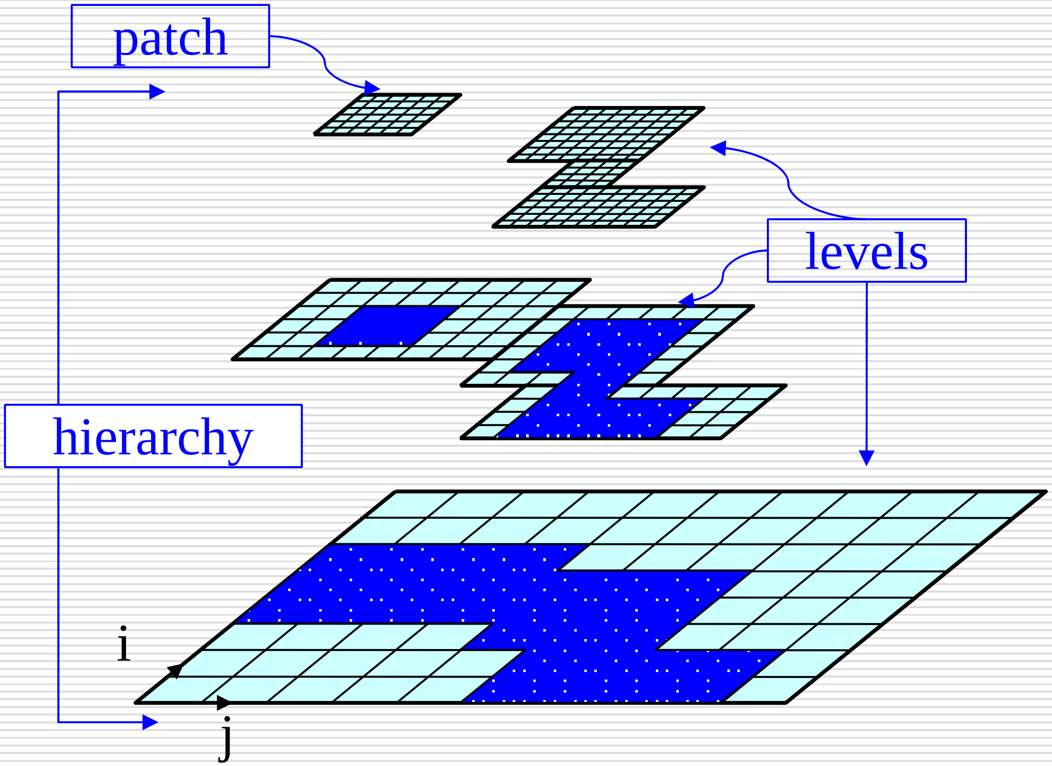
ALE-Lagrange

Corrector

1. Compute the acceleration using the momentum equations: anp1=f(xp,pp,sp,qn,h)/m
2. Integrate the velocity: unp1=un+0.5*dt(an+anp1)
3. Integrate the node positions: xnp1=xn+0.5*dt*(un+unp1)
4. Compute the strain rates: r=f(un,unp1,xn,xnp1)
5. Compute the volume Vnp1 and densities: dnp1=dnVn/Vnp1
6. Compute the energies: enp1=f(pn,pnp1,qn,sp,r,h,Vn,Vnp1)
7. Compute the stresses:snp1=f(sn,Vn,Vnp1,r)
8. Compute the pressure:pnp1=f(dnp1,enp1)

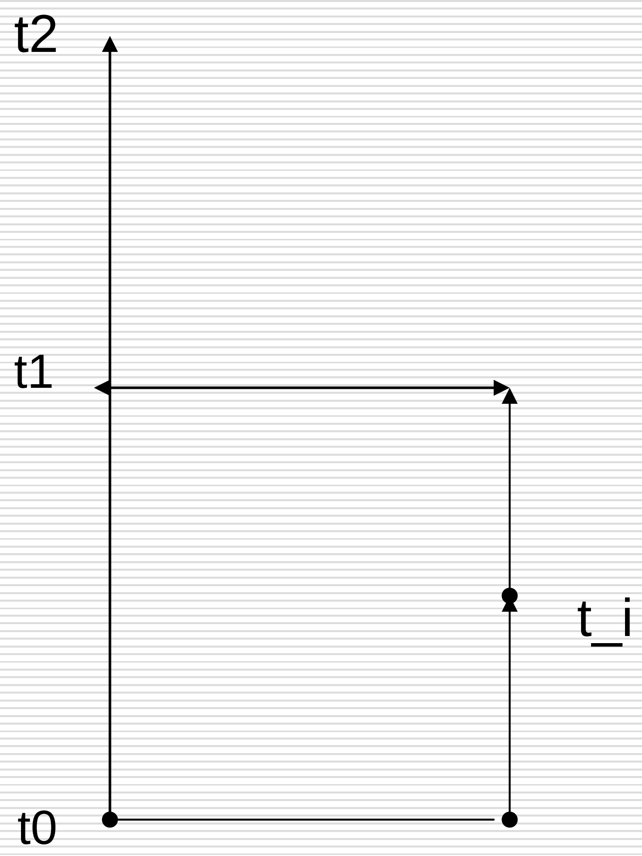
Dynamic AMR

- Berger-Oliger-Colella AMR
- Dynamic
- Geometrically flexible
- Efficiency
- Complexity of data structure
- Data management



AMR hierarchy integration

- Solutions advance to a level
- Coarse grid advances
- Multiple fine grid advances
- Solution synchronization between levels



ALE-AMR: technical approach

- Using SAMRAI tool to manage the basic data structure for AMR and parallel computation.
- Focus on numerical methods and solution algorithms to design ALE-AMR.
- Interlevel transfer operators.
- Coarse-fine boundary conditions.
- AMR on a moving mesh.
- Criteria of refinement and coarsening.

ALE-AMR : technical approach

Interlevel operators design goals:

1. Constant field preservation.
2. 2^{nd} order accuracy.
3. Monotonicity.
4. Local conservation.
5. Exact inversion of refinement by coarsening.
6. Positivity preservation.

ALE-AMR : technical approach

Interlevel transfer operators

- Second order interpolation from coarse grids to fine grids

$$\phi(x,y,z) = \phi_0 + \phi'_{x0}(x - 0.5\Delta x_0) + \phi'_{y0}(y - 0.5\Delta y_0) + \phi'_{z0}(z - 0.5\Delta z_0)$$

The primitive variables and the basis are

$$\phi = (\rho, u, v, w, E, s, p)$$

$$x = (V, \tilde{m}, \tilde{m}, \tilde{m}, m, V, V)$$

ALE-AMR : technical approach

Local conservation :

$$\sum_{i,j,k}^{r1,r2,r3} \phi^I X^I = \phi^{I-1} X^{I-1}$$

If the basis consistency condition holds:

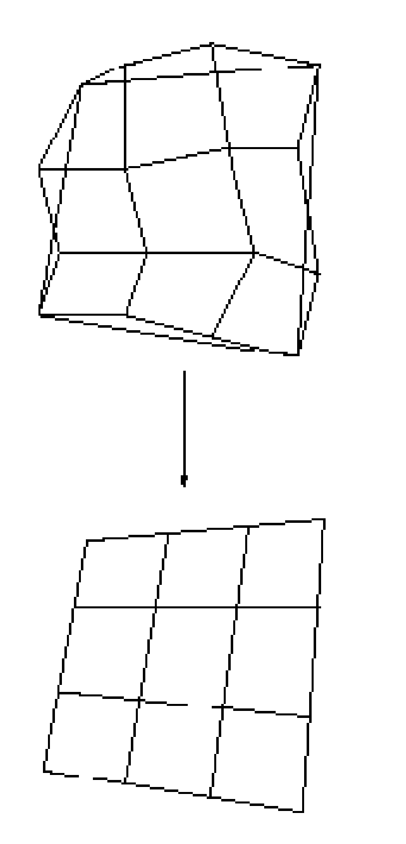
$$\sum_{i,j,k}^{r1,r2,r3} X^I = X^{I-1}$$

ALE-AMR: technical approach

- Coarsening operators

$$\rho 0 = \frac{\sum \rho_i V_i}{\sum Vi} = \frac{\sum \rho_i V_i}{V_0}$$

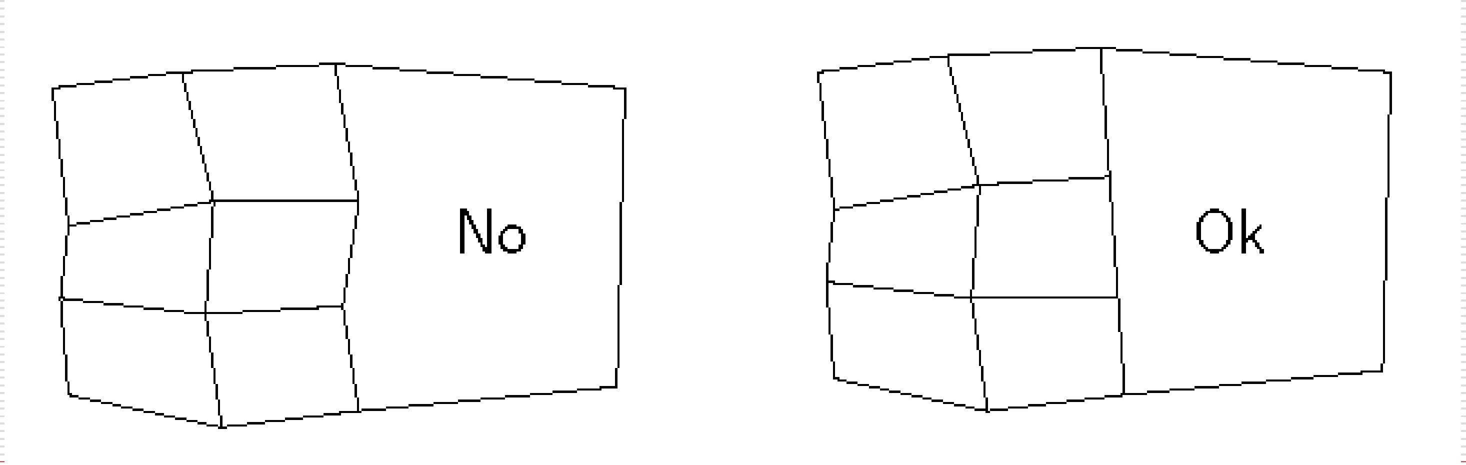
$$S_0 = \frac{\sum SiVi}{\sum Vi} = \frac{\sum SiVi}{V_0}$$



The property holds for other variables as well after a preprocessing remap step to an aligned grid .

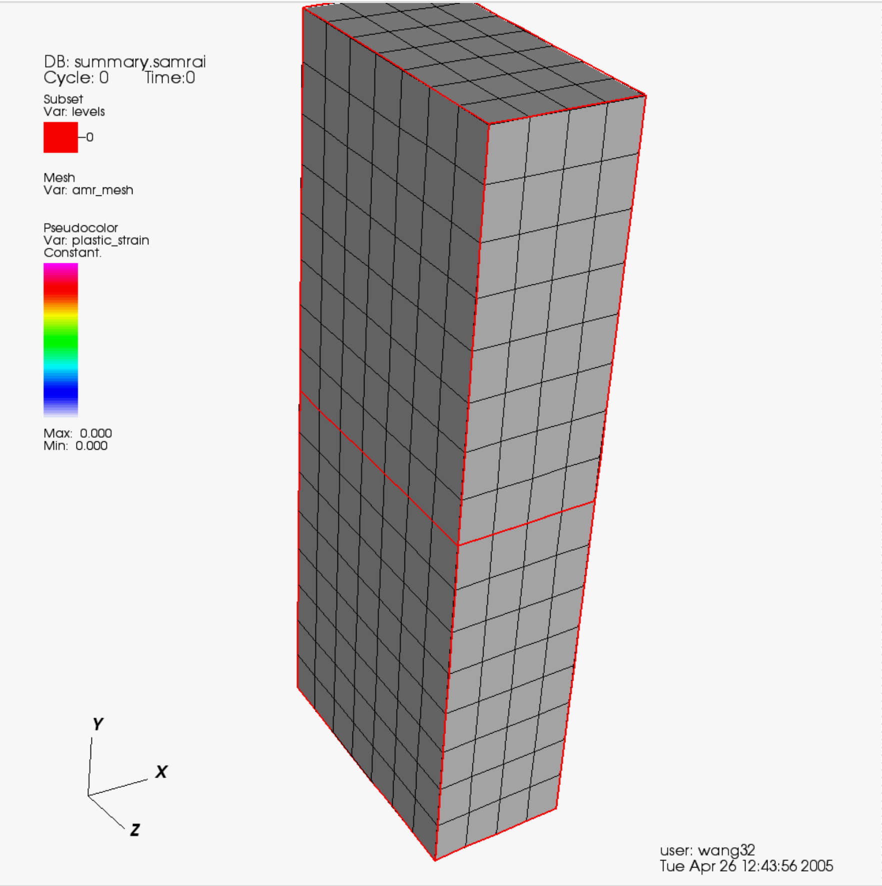
ALE-AMR: technical approach

- Coarse-Fine Boundary Conditions
- Position of coarse-fine boundary nodes linearly interpolated in time and space
- No nonhex/nonquad elements on a composite mesh

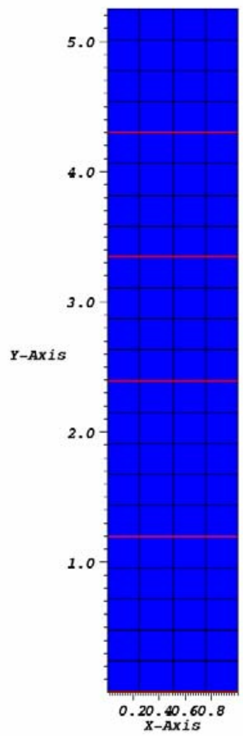


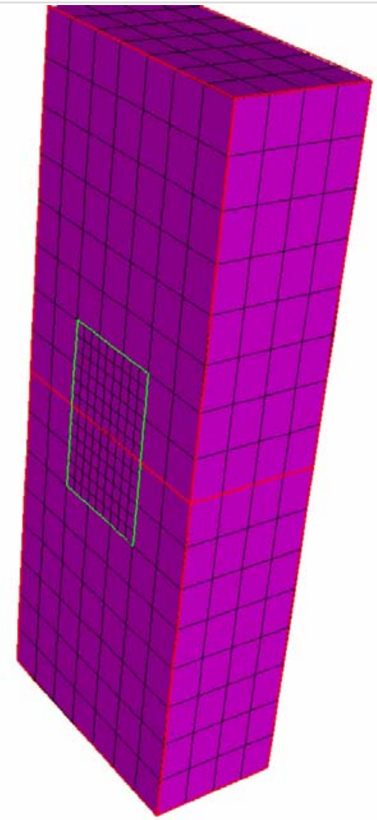
Results and discussion (elastic flow)

- For perfect elastic flow, we have tested several vibration beams problems which can be readily checked by elasticity theory.
- Simulation of the vibration plates with two fixed ends.
- Vibration motion is expected from the simulation.

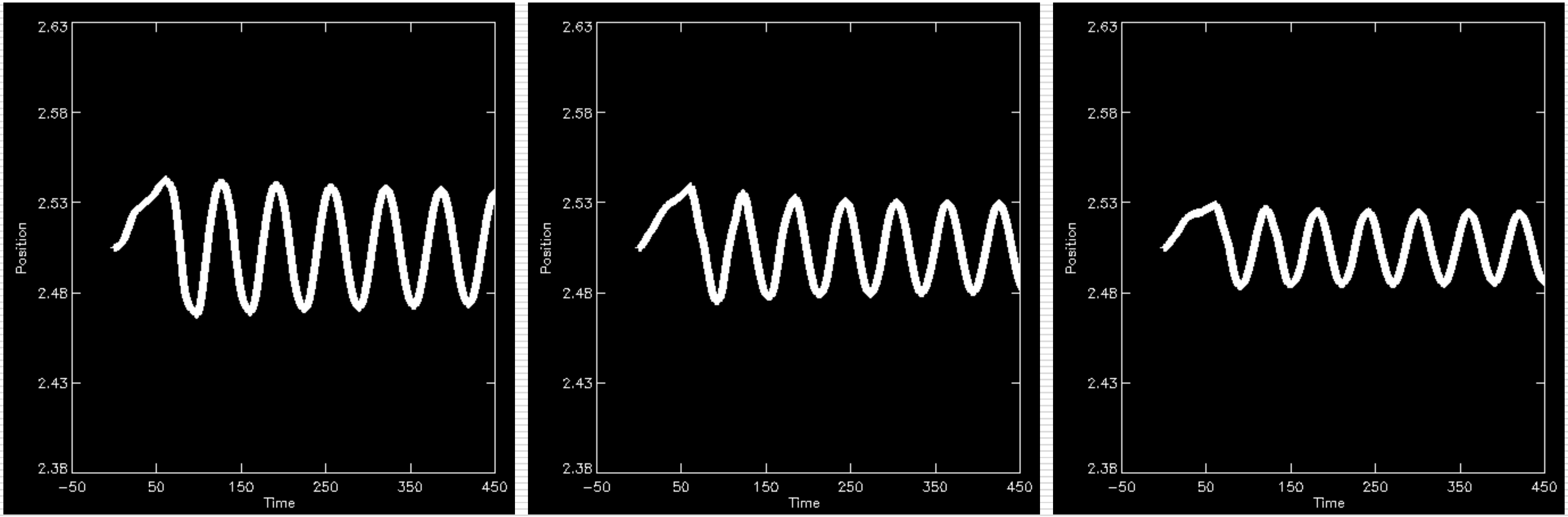


Results and discussion-2D and 3D vibration plates (elastic flow)





Results and discussion-vibration plates

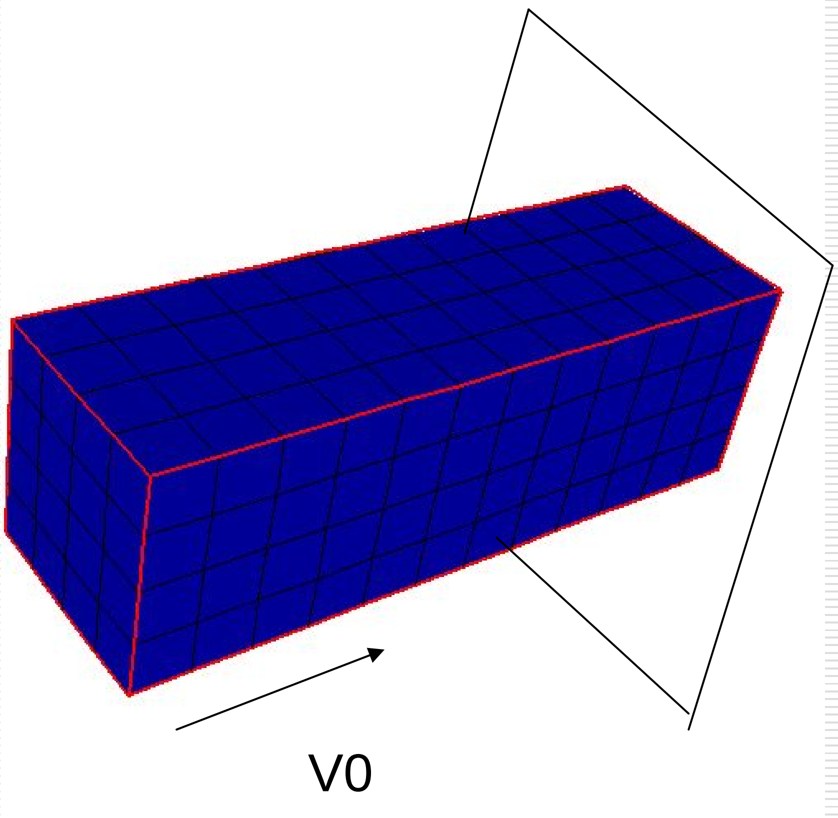


(a) (b) (c)

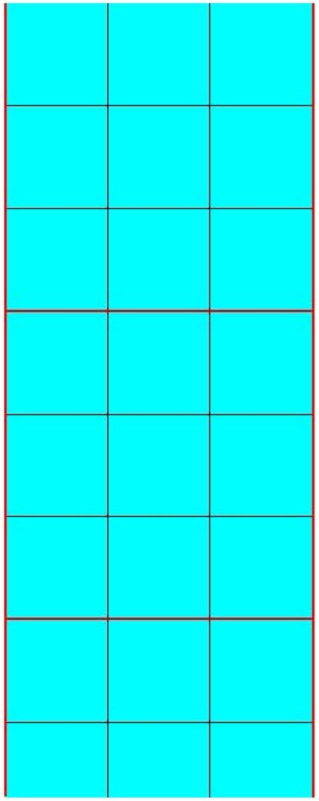
Frequency of 2D vibration plate is check by elasticity theory with different resolutions (a) 2x12, (b) 4x24, and (c) 8x48.

Results and discussion (elastic-plastic flow)

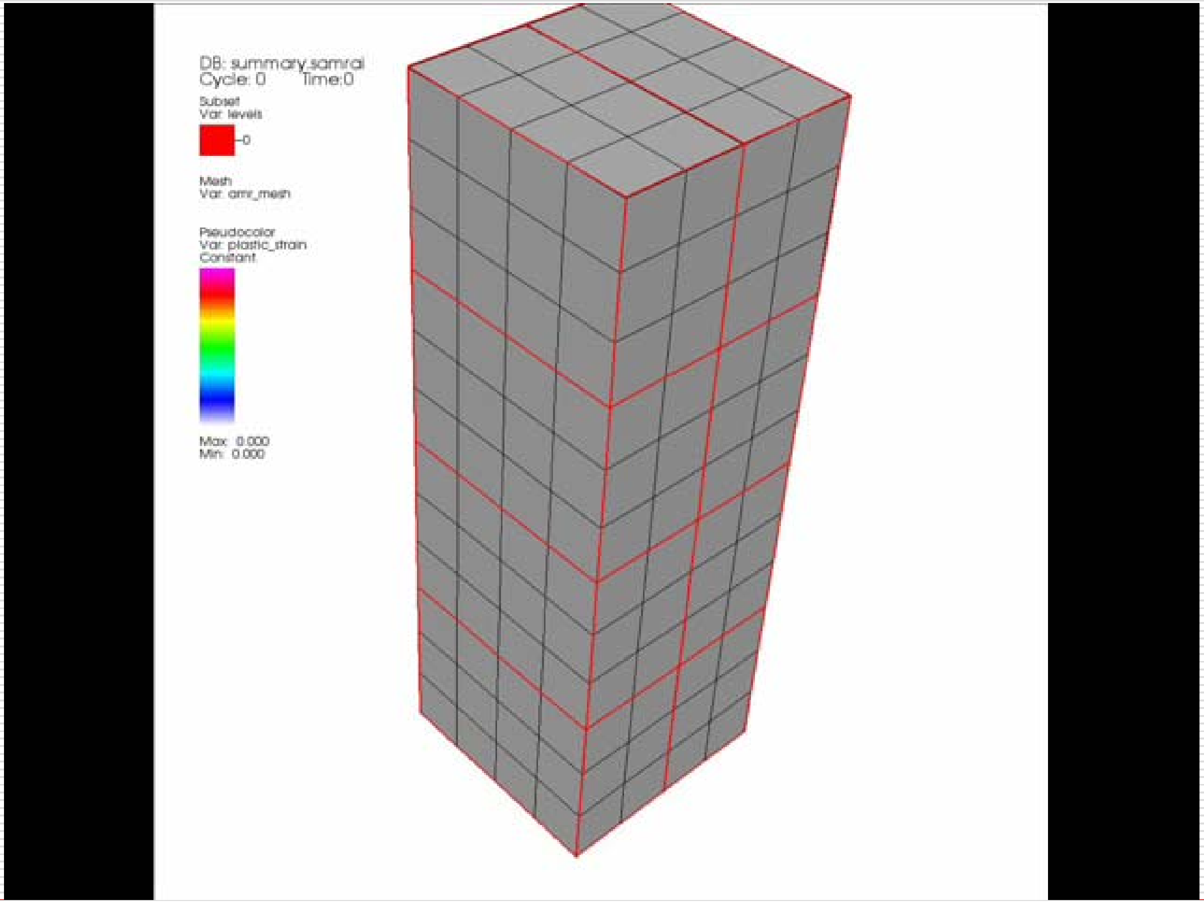
- Elastic-Plastic flow problem set up
- Simulation of the impact of an extruded rectangular solid of metal material on a rigid wall
- Plastic deformation is expected from this motion



Dynamic ALEAMR 2D in motion-elastic-plastic flow)



Dynamic ALEAMR 3D in motion (elastic-plastic flow)



Dynamic ALEAMR 3D for failure and fragmentation predictions-problem 1

Problem 1: Tantalum ring (34.37 mm inside diameter, 35.89 mm outside diameter and 0.76 mm thick) with velocity applied at the inner boundary.

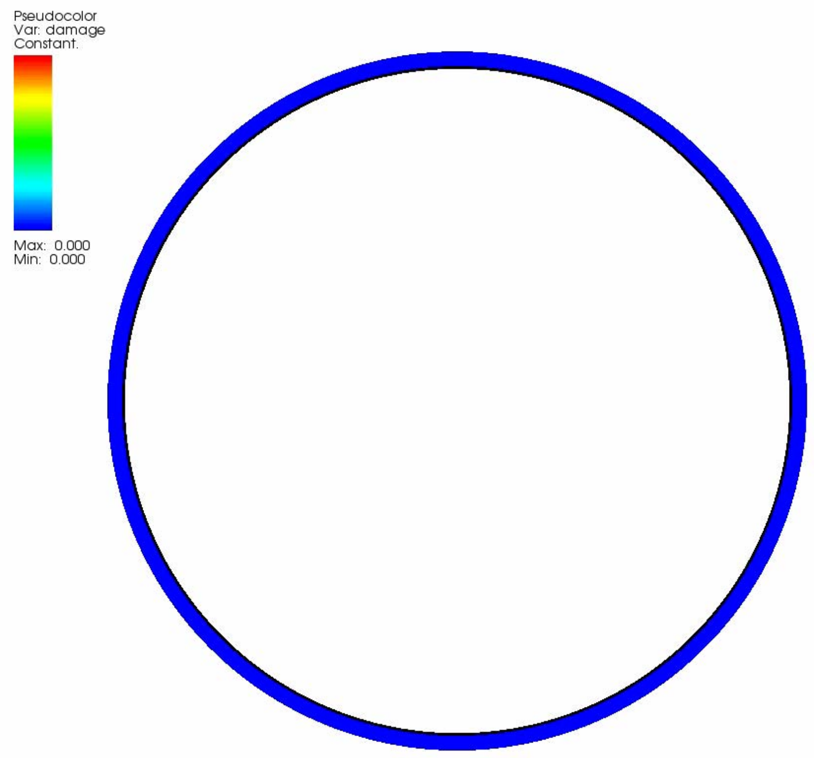
Failure model: Johnson-Cook failure model.

Mesh: 5x5x600

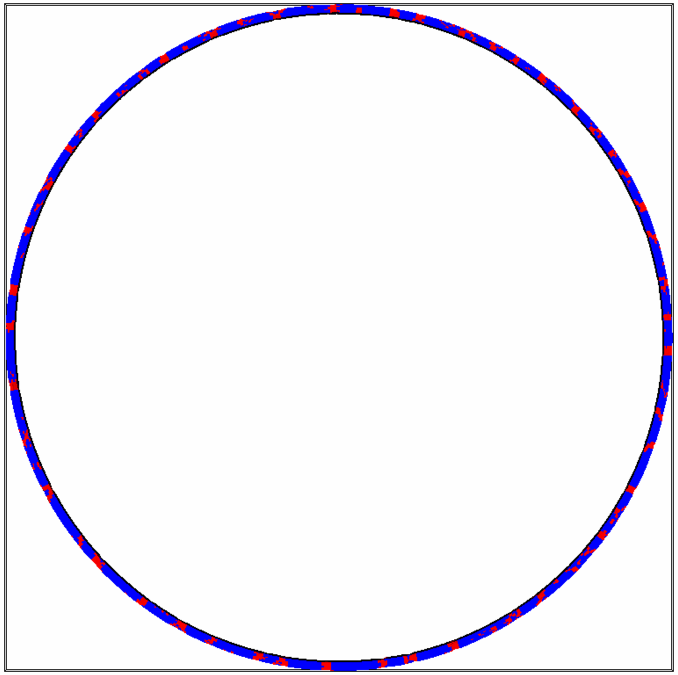
Velocity: on inner surface

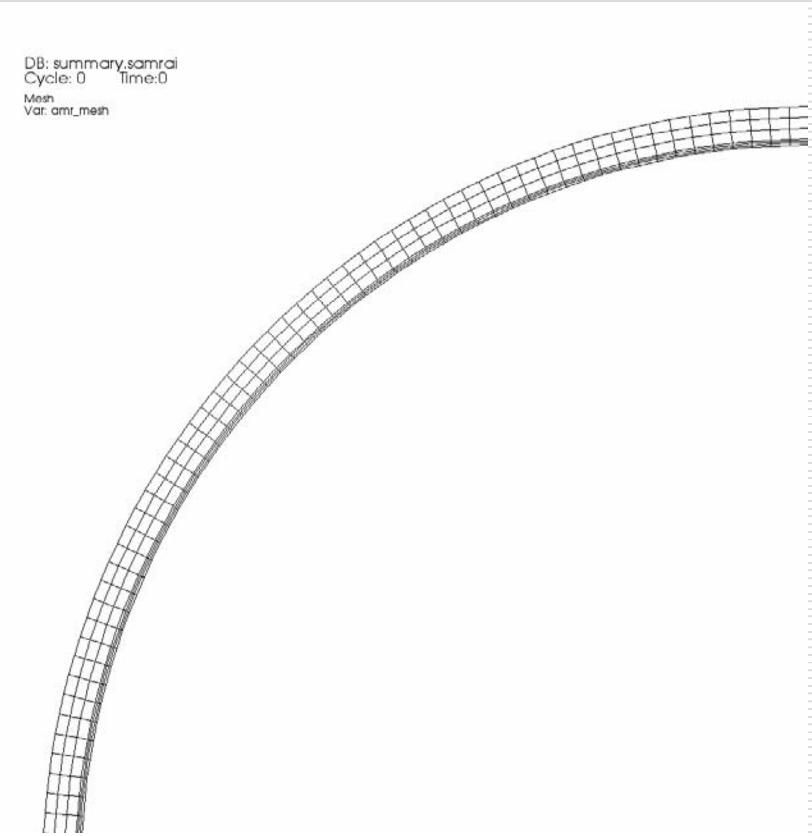
v= 0.03 X t/12 {cm/ms}

for t = 0-12 ms

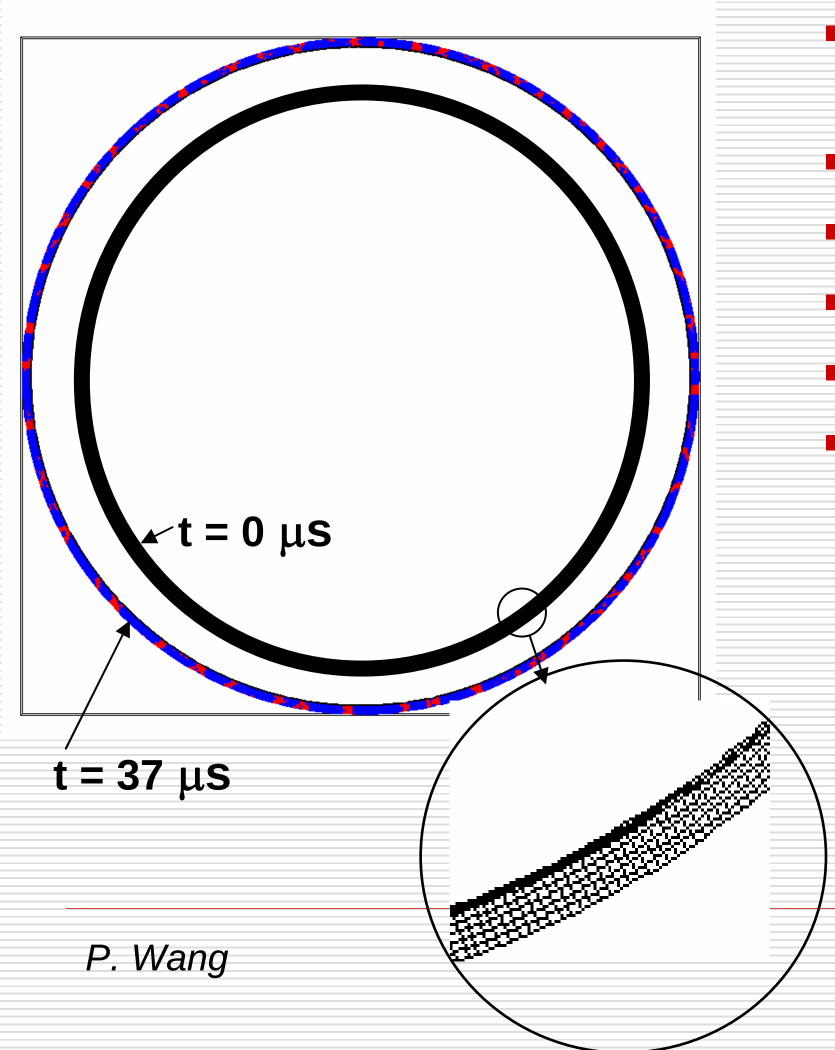


Dynamic ALEAMR 3D for failure and fragmentation predictions





Material strength and failure models



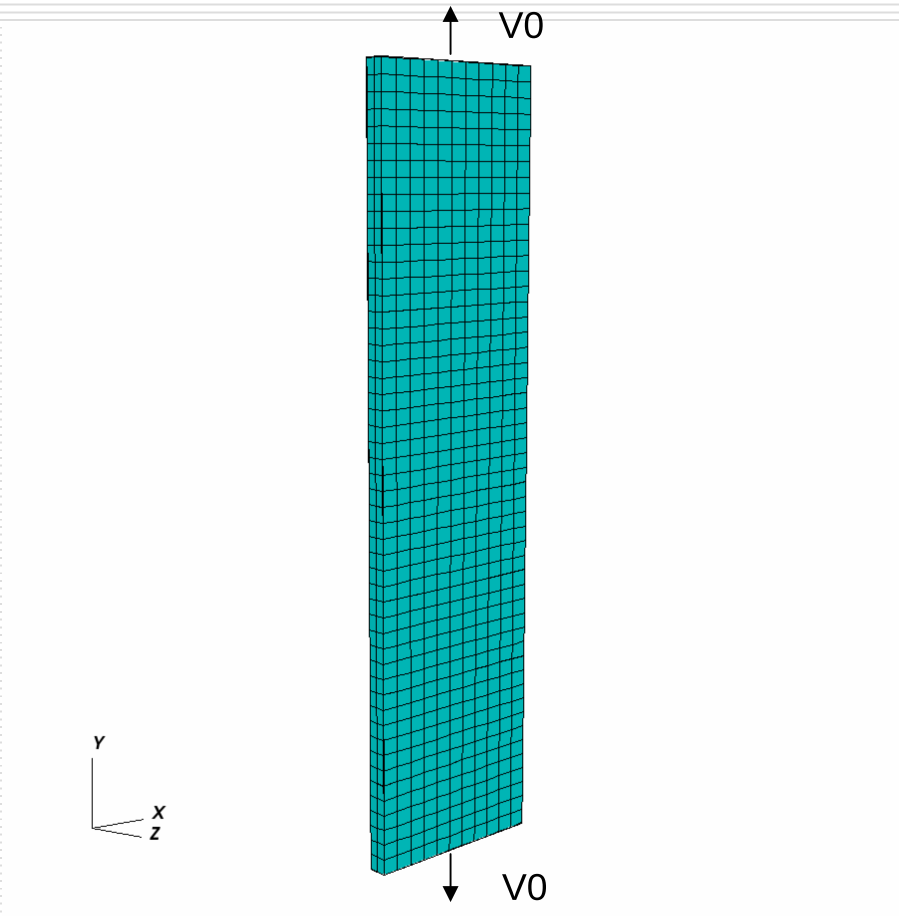
- 3D ALE-AMR test case of Ta expanding ring
- Lagrangian hydrodynamics
- Johnson-Cook model with Failure
- Ring expands and thins
- Red denotes material that has failed
- Time of failure and number of fragments agree with the experimental data (Niordson 1965,Olson 2002) and the numerical data (Becker 2002) from other codes.

Dynamic ALEAMR 3D for failure and fragmentation predictions-problem 2

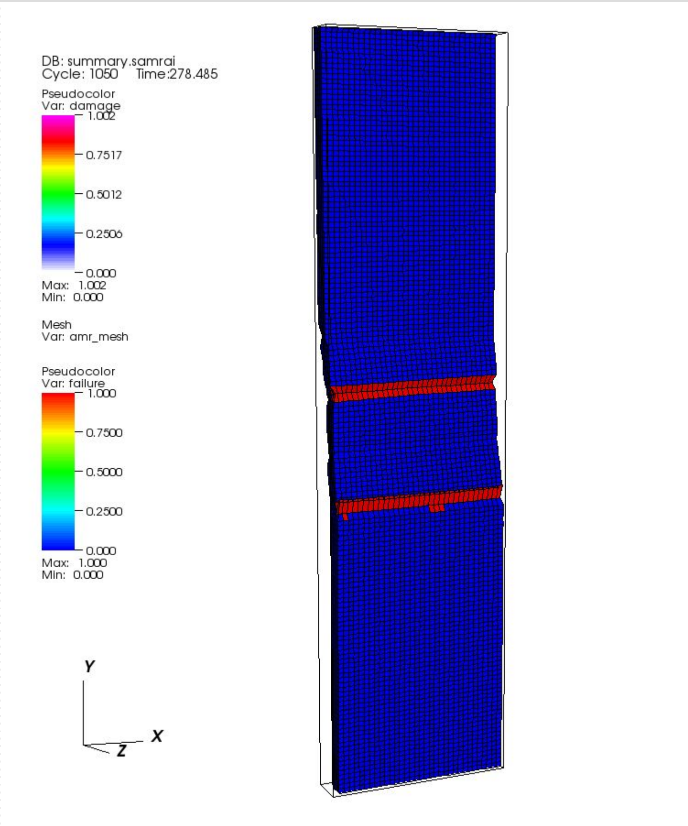
Problem 2: Tantalum thin plate (5.0 cm x 20.0 cm x 0.2 cm) with velocity applied at the two ends.

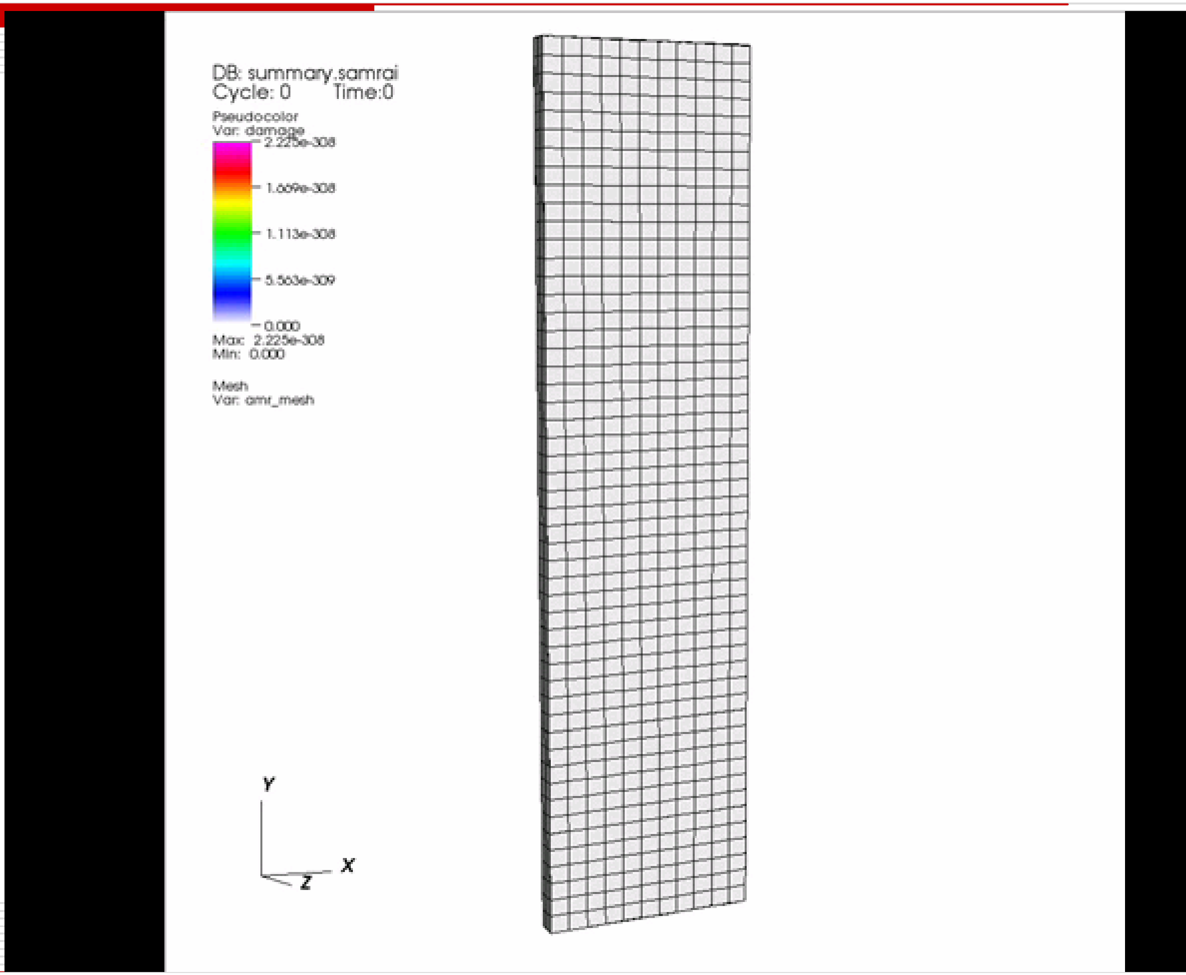
Failure model: Johnson-Cook failure model.

Mesh: 11x51x2 with 2-levels AMR mesh.



Problem 2 : Numerical simulation results of the damage and failure fields

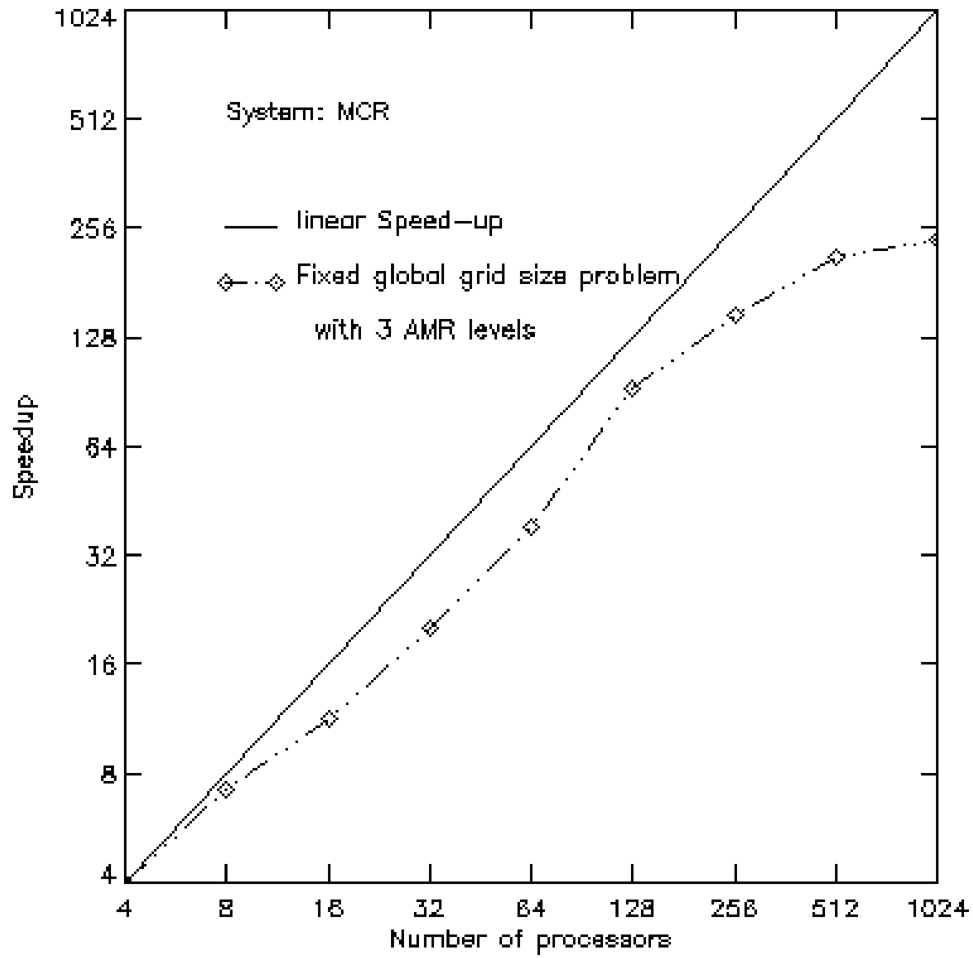




Parallel performance

- Parallel performance: fixed global size problem: 16x64x16 with 3 levels AMR (about 300k total grid points, it ranges 75000 to 300 grid points from 4 cpu to 1024 cpus).
- System: MCR a Linux cluster: 1112 dual nodes with 2.4 GHz for each cpu.

Parallel performance for the fixed global size problem



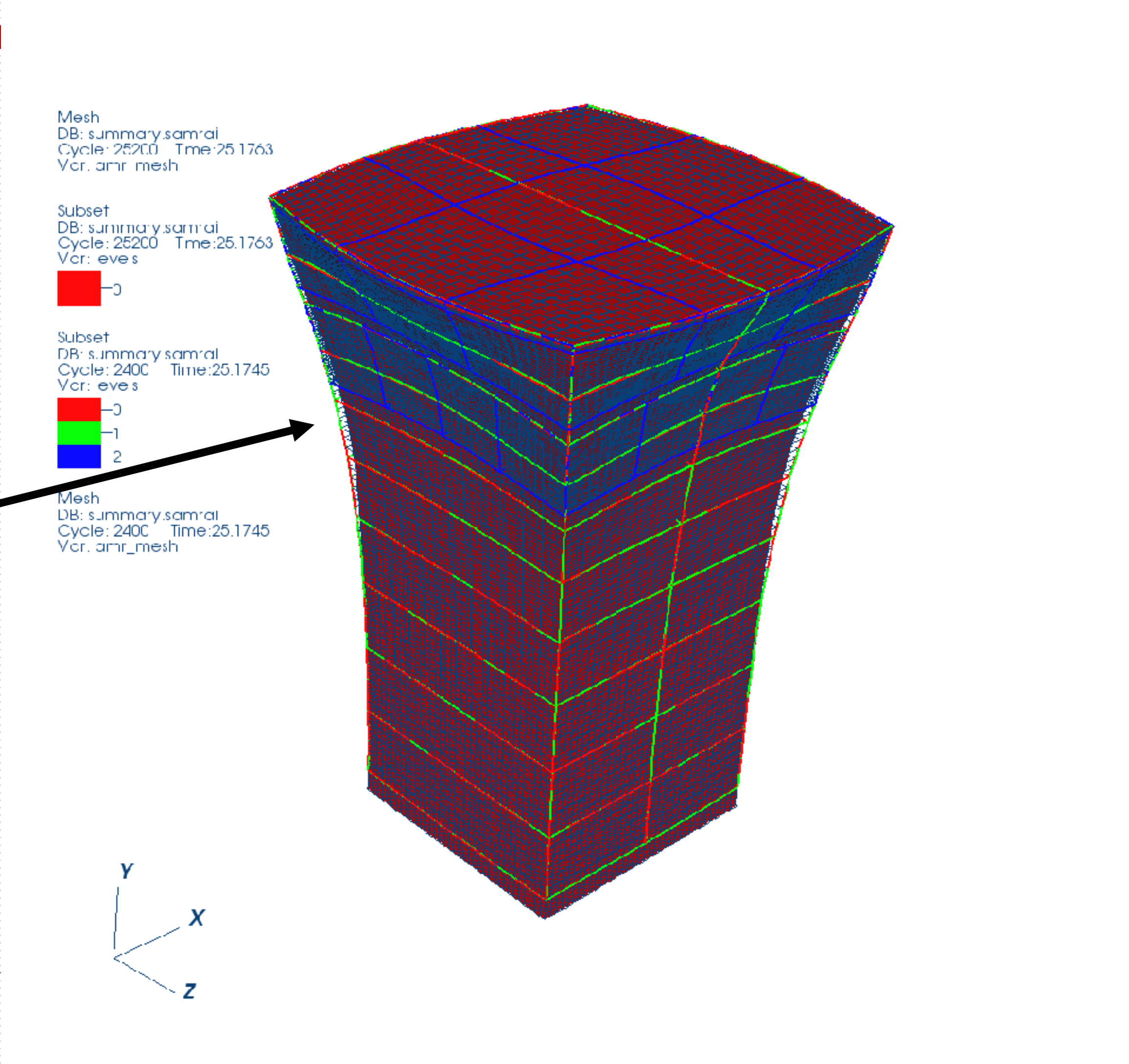
Efficiency study of the ALE-AMR Algorithm

Impact problem at 25 μs	Single mesh	AMR mesh	Differences
Total CPU time (s) on MCR with 16 processors	39145	22155	41%
Maximum plastic strain	1.186	1.198	1%

Computational efficiency and accuracy comparisons between the results from a single mesh 36x180x36 and the one from a 3-level AMR mesh with an initial coarse mesh 4x20x4.

Results from a single mesh and a 3-level AMR mesh at 25 μs

AMR mesh (gray)



Conclusions

- A new numerical method combining ALE with AMR is developed.
- The ALE-AMR method has been applied to several problems in hydrodynamics and material modeling, and the method shows excellent computational efficiency.
- The method shows good scalability on a large number of processors.
- The method shows the great potential to attack complex problems : multi-scale modeling which allows simulation over a large range of time or distance scales that are currently modeled by separate codes and methods.

Work under investigation and future directions

- More material failure and fragmentation simulations with ALE-AMR.
- Apply our current work to complex problems.
- Multi-physics simulations (radiation, multi-materials and others).
- Verification and validation with experiments.

Acknowledgements

Bob Anderson

Rich Becker

Alice Koniges

ALE-AMR and SAMRIA teams

NIF Mission Support Team

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.